Predicting Deformation and Cracking as a Function of Additive Manufacturing Process Parameters

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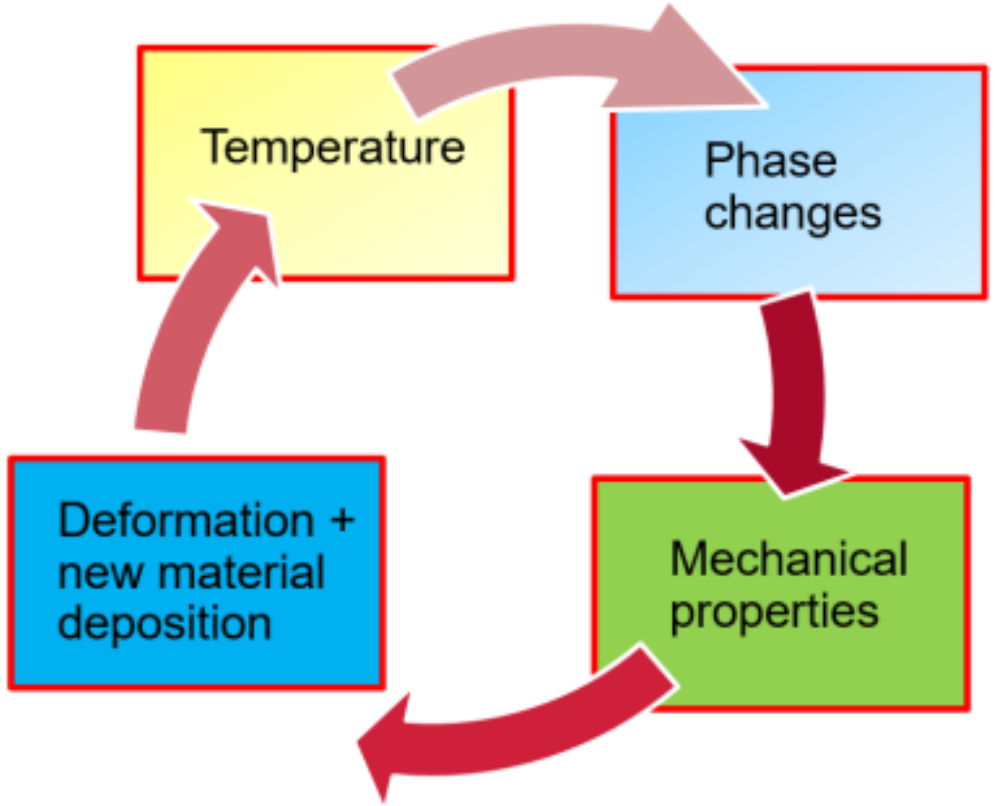
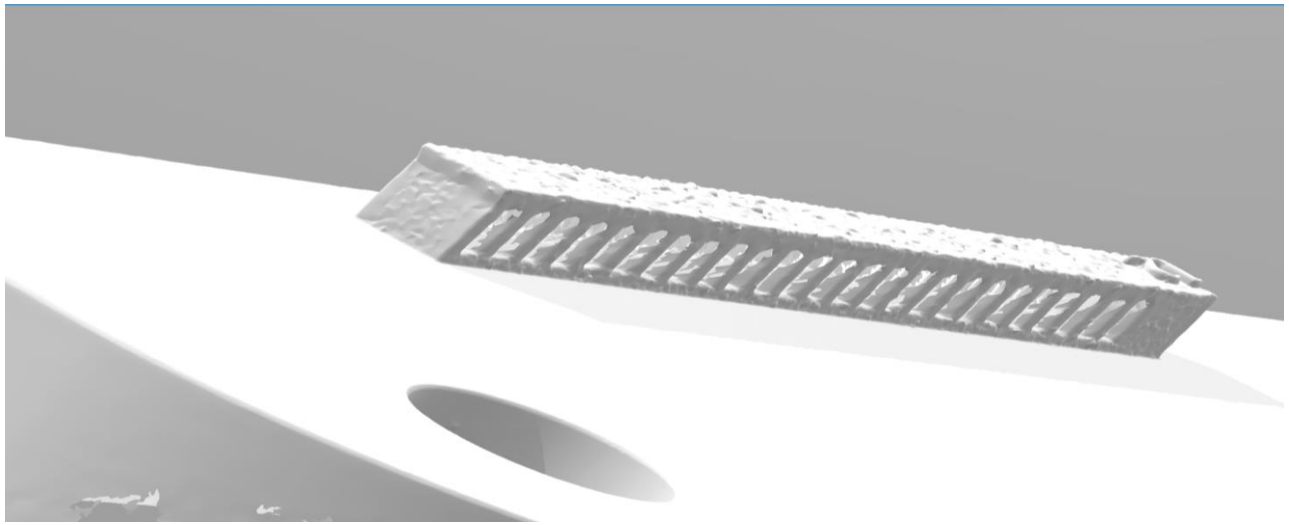
Technical Approach

- **Combine:**
  - **Part-level FEM model of residual stresses**
  - **CALPHAD-based phase transformation model for precipitation of brittle phases**



JPL FEM Model Features

- Element Progressive Activation (EPA)
- Surface film (FFS) and radiation (RFS) capabilities
- Non-uniform heat flux in 3D heat transfer
- Elements are switched on and off at specific times



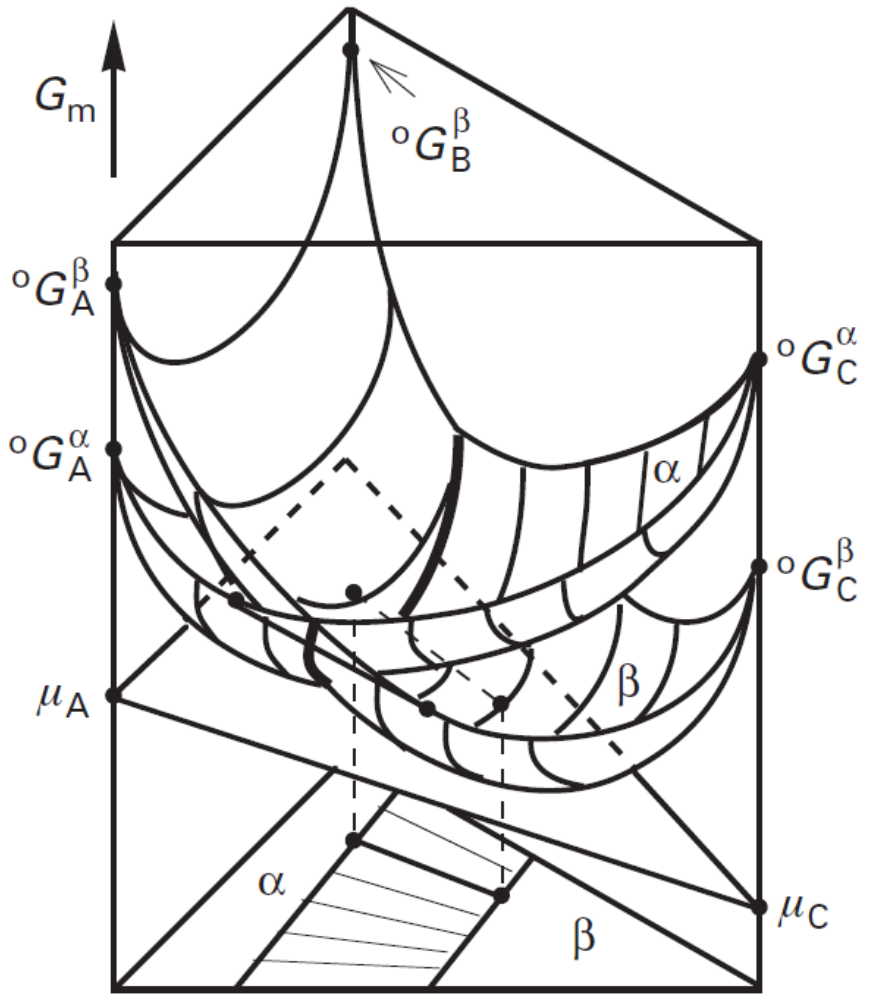
CALPHAD

Phase-based modeling of material properties – equilibrium and non-equilibrium

$$\min G(T, P, f_i, y_j^s)$$

$$G_m^{\alpha}(T, x_i) = \sum_i x_i(\Delta G_i^{\beta, 298.15 \to T} + \Delta G_i^{\beta \to \alpha} + RT \ln x_i) +$$

$$\sum_{i,j} x_i x_j \sum_m {}^m L_{i,j}(x_i - x_j)^m + \sum_{i,j,k} x_i x_j x_k (x_i I_i^{i,j,k} + x_j I_j^{i,j,k} + x_k I_k^{i,j,k})$$



Hillert, 2007

IP[y]: Notebook BinaryExamples Last Checkpoint: Jan 08 23:25 (autosaved)

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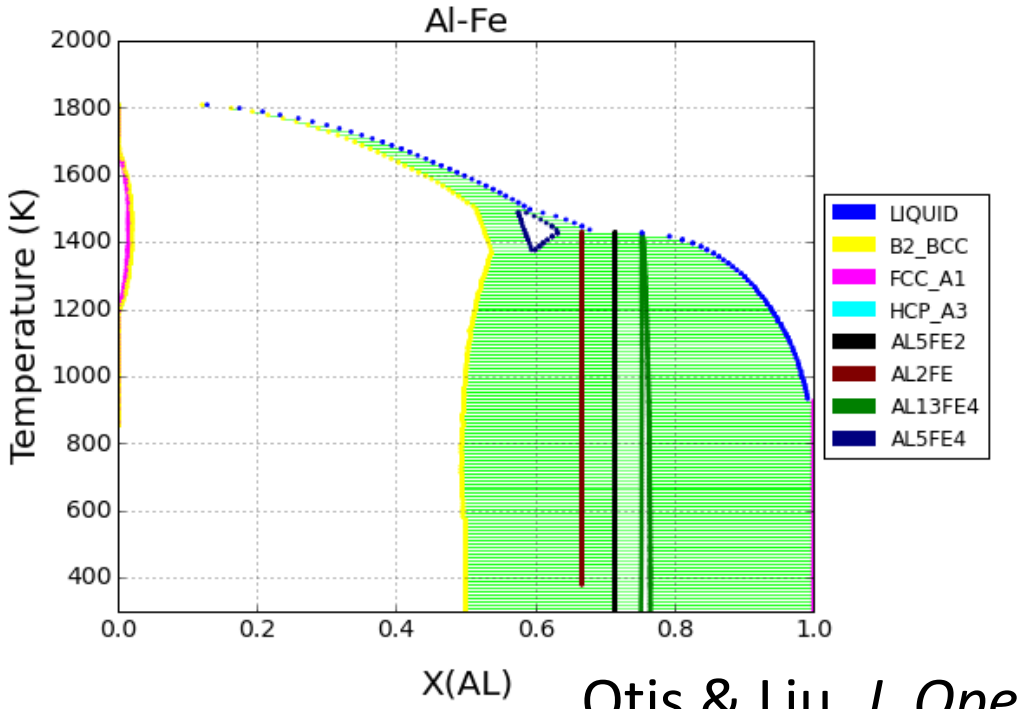
Al-Fe (M.Seiersten et al., 1991)

In [3]:
```
db_alfe = Database('alfe_sei.TDB')
my_phases_alfe = ['LIQUID', 'B2_BCC', 'FCC_A1', 'HCP_A3', 'AL5FE2', 'AL2FE', 'AL13FE4', 'AL5FE4']

fig = plt.figure(figsize=(9,6))
pdens = [{'B2_BCC': 20000}, 2000]
%time ax = binplot(db_alfe, ['AL', 'FE', 'VA'] , my_phases_alfe, 'X(AL)', 300, 2000, pdens=pdens, ax=fig.gca())
plt.show()
```

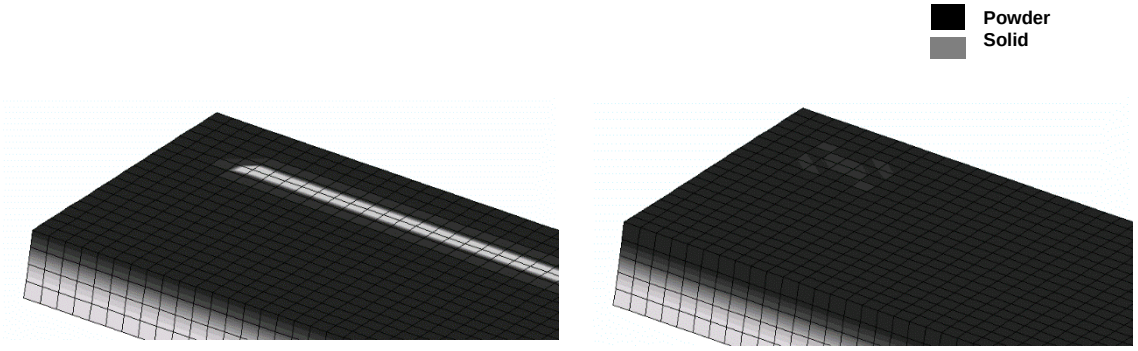
```
CPU times: user 27.5 s, sys: 639 ms, total: 28.1 s
Wall time: 17.1 s
```



pycalphad.org
- Open source CALPHAD tool
- Supports user-supplied phase models

Otis & Liu, *J. Open Res. Softw.* **5,** 1 (2017).

FEM Simulation of Residual Stress

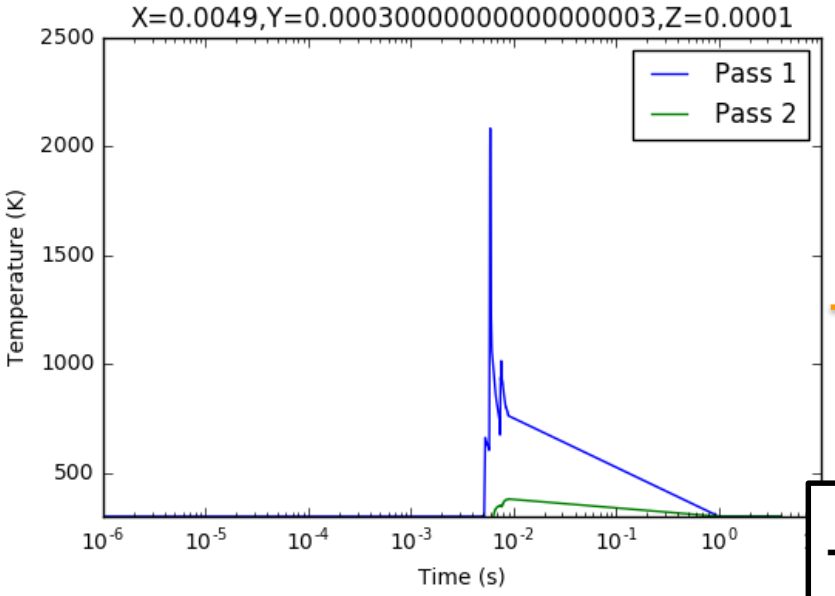


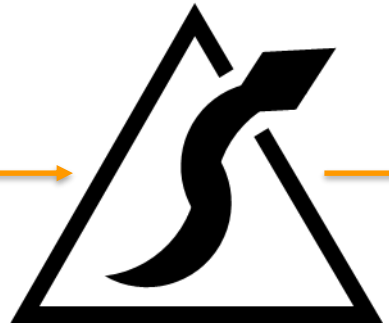
Step 1
Three solid layers

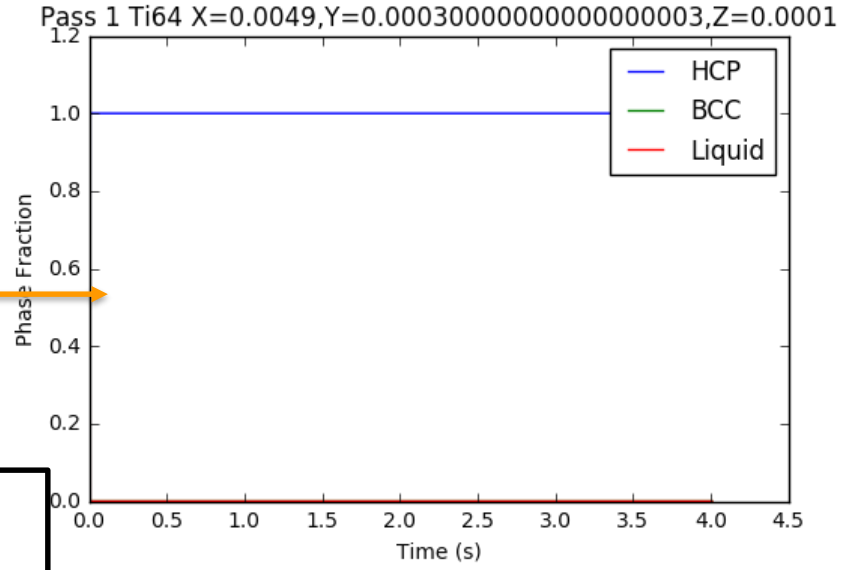
Step 2
Four layers: one powder layer with sintered line on top of three solid layers

Step 3
Five layers: one powder layer on top of four layers from previous step

FEM-CALPHAD Integration



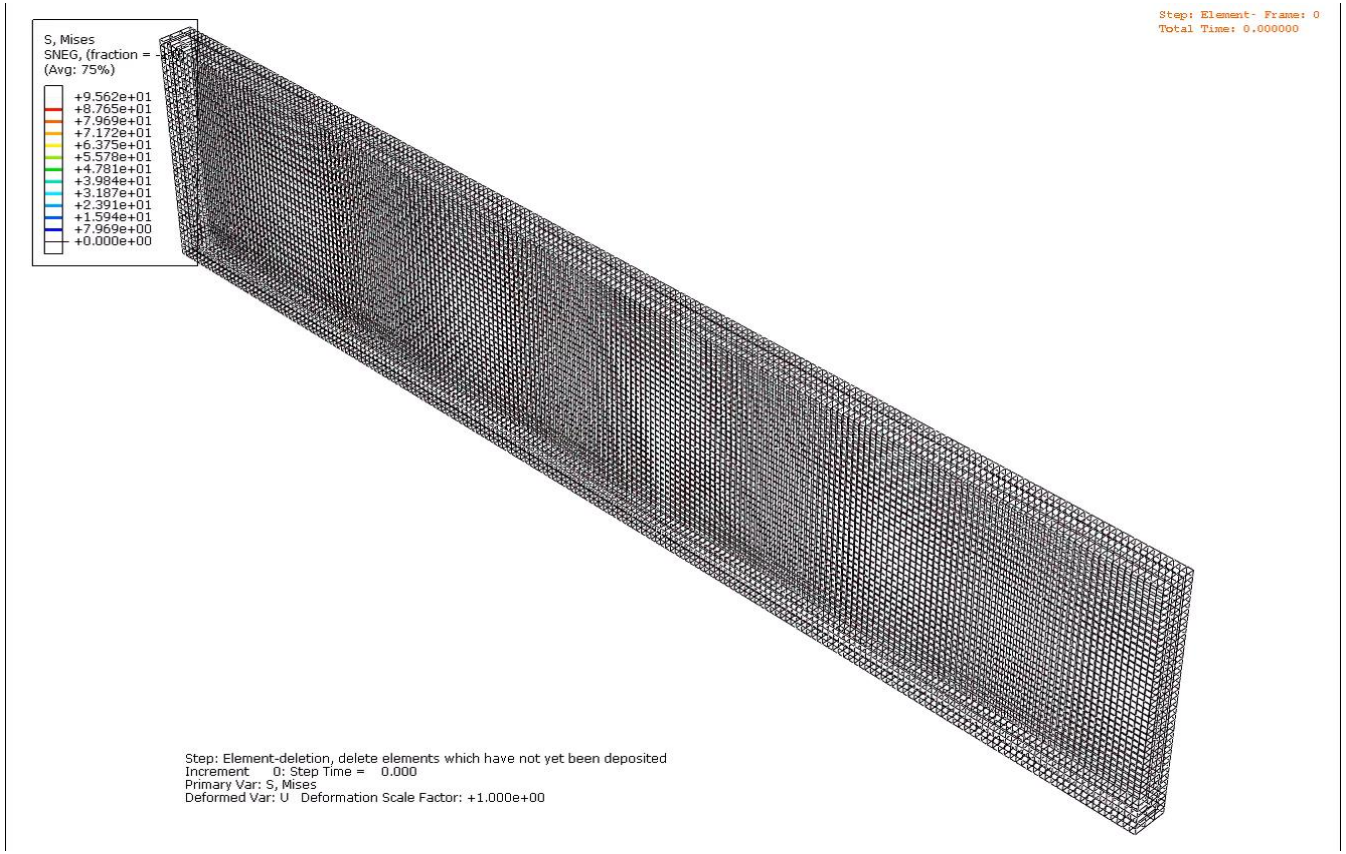




Test on using Ti64 FEM temperature profile to predict phase fractions

This shows the flow of data is working

Residual Stress Movie



NASA ARC: Whole part modeling in COMSOL

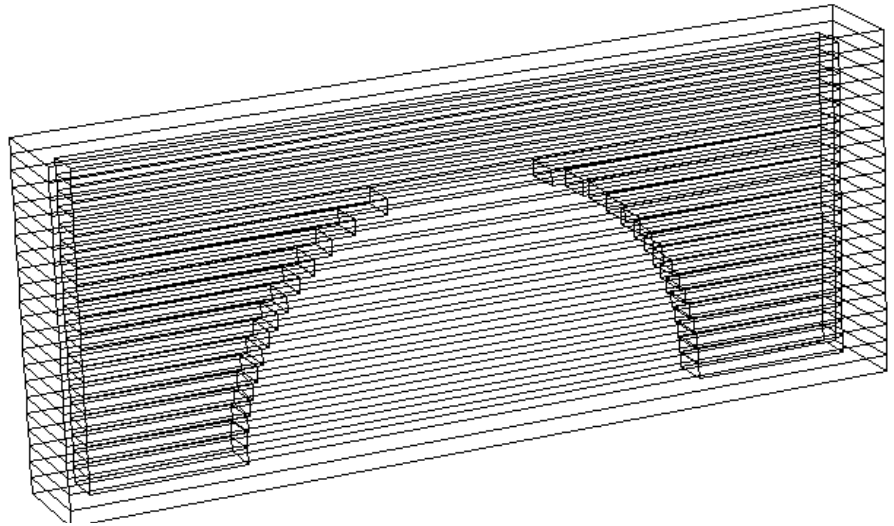
Geometry created in Python script with COMSOL primitives

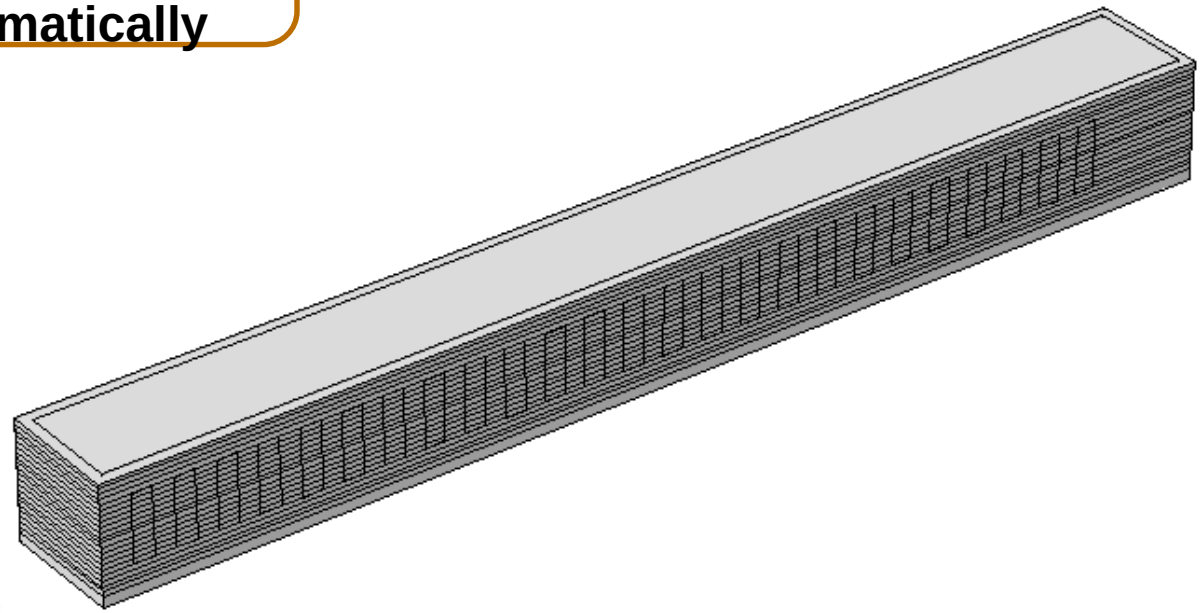
Python code generates files readable by COMSOL as separate models

B.C.s change with each layer automatically

Scripts call each model/layer in turn with initial conditions of thermal and structural results from last layer

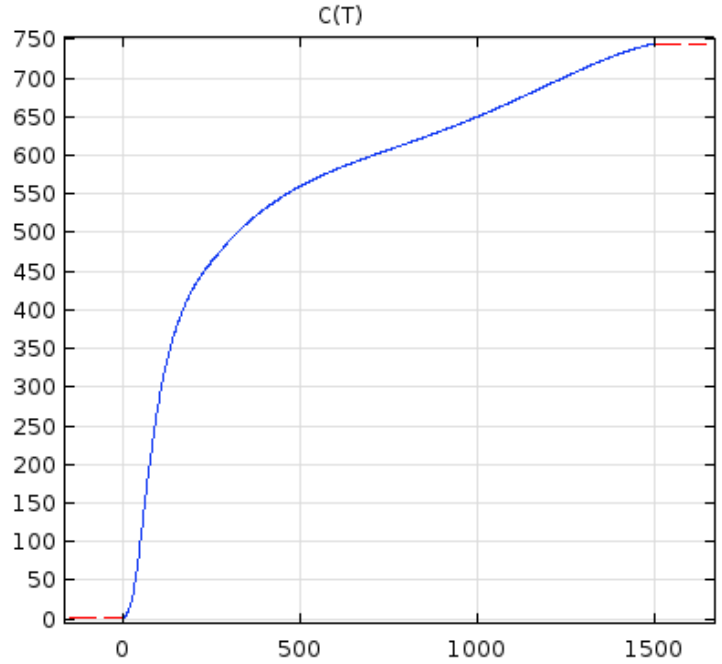
Temperature field data from each layer fed to pycalphad





Relevant physics incorporated in COMSOL

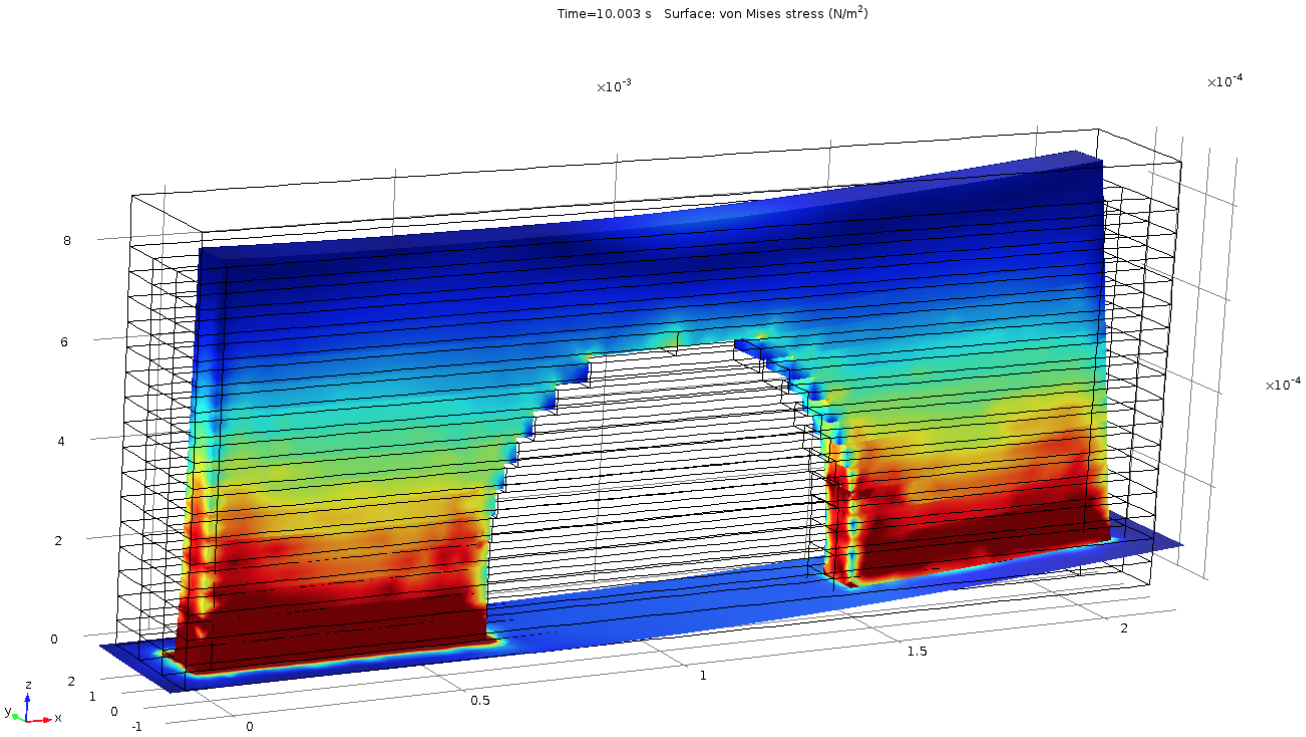
- Solid Mechanics
  - Stress
  - Strain
- Heat transfer
  - Phase changes from solid to melt to vapor
  - Evaporation
  - Radiation from surface
  - Boundary heat source for laser
- Material Properties
  - Fully non-linear temperature dependent properties for 316LSS and IN718

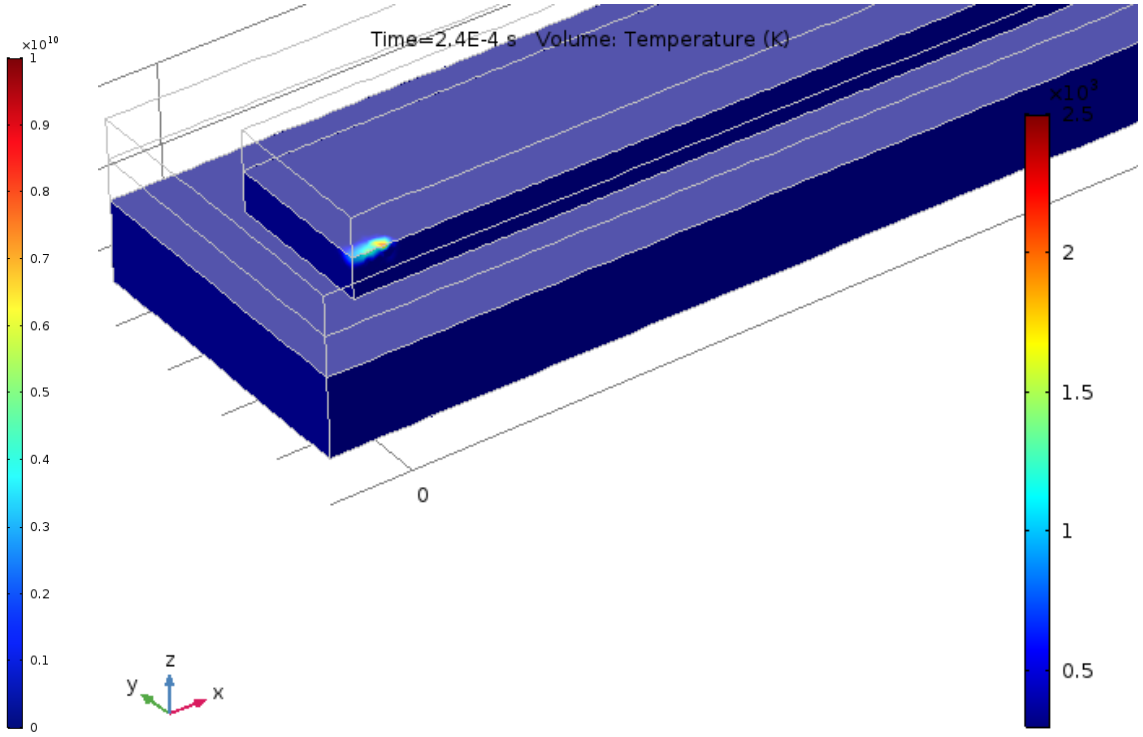


COMSOL Results for additive SLM

Models of layer by layer build process predict expected angles of distortion due to residual stress

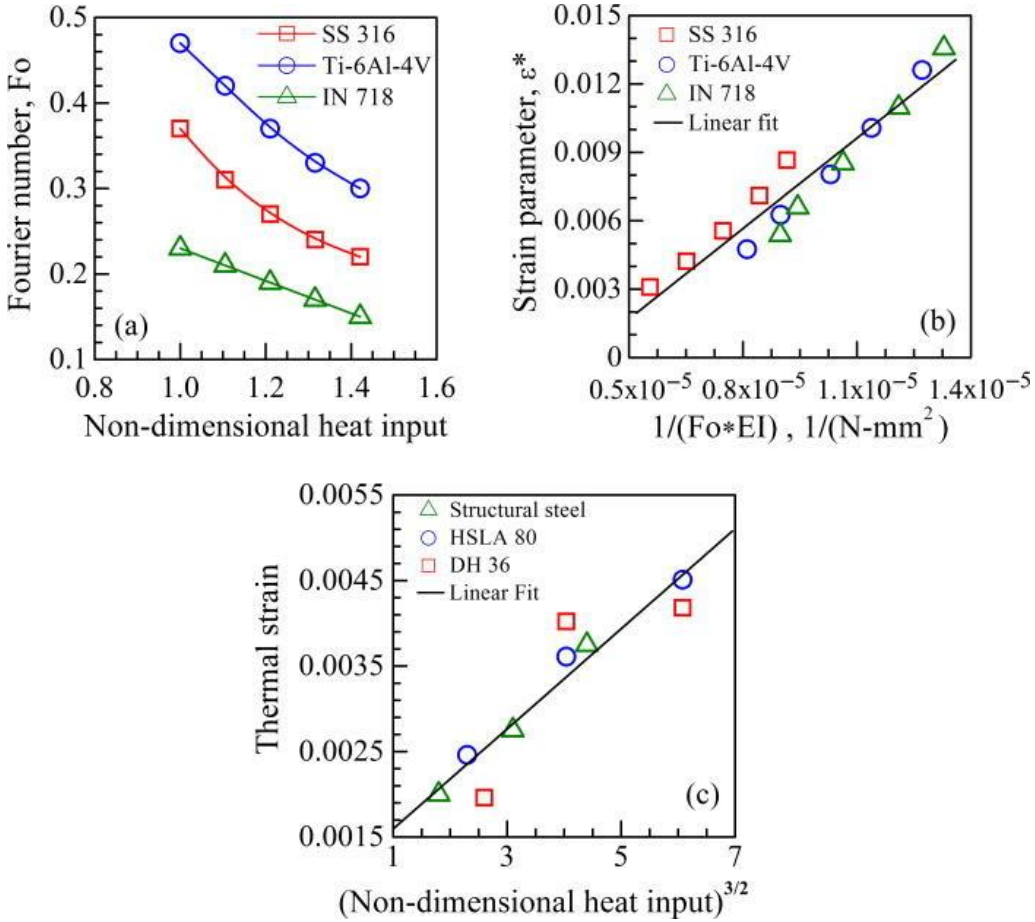
Models of thermal process can provide temperature profiles over space and time to CALPHAD





Future Work: Reduced-Order Models

- For AM process design, many iterations will be required
- FEM is not feasible to run in a tight design loop
- One option: “scaling” relations



T. Mukherjee; V. Manvatkar; A. De; T. DebRoy; *Journal of Applied Physics* 2017, 121